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Pseudopotential operator for hard-sphere interactions in any-dimensional space

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The quantum-mechanical two-body problem with hard-sphere interaction in any-dimensional space is studied by means of Fermi's pseudopotential. A unified pseudopotential operator is obtained for the interactions in different space dimensionalities.

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Although the properties of a Bose system have been studied for decades, the experimental achievements [1–3] on Bose-Einstein condensation (BEC) have stimulated a renewed surge of theoretical investigations on this system. A massive literature is devoted to the effects of interactions on the ground state of a Bose gas (see, for example, Refs. [4–7]) on excitations of the condensate (see, for example, Refs. [7–10]) and on the critical temperature (see, for example, Refs. [11–13]). However, a majority of these studies is based on the mean-field approximation and considers only the case in three-dimensional (3D) space. On the other hand, some authors [14–16] have investigated the effects of space dimensionality, however, just for ideal Bose gases. It is worth pointing out that two-body interactions are expected to modify in a deep way the behavior of the phase transition in different space dimensionalities.

In order to facilitate discussion of imperfect Bose gases in different space dimensionalities, the quantum-mechanical two-body problem with hard-sphere interaction in any-dimensional space is studied by means of Fermi's pseudopotential to obtain a generalized pseudopotential operator.

In view of the low temperature and density conditions present in the experiments, it is a good approximation to take into account only the S wave and include only the scattering length a, ignoring the higher partial waves and excluding the S-wave parameters beyond the scattering length, i.e., to calculate to the order a. Thus interaction between atoms is well characterized by hard-sphere interaction with a pseudopotential operator [17]

$$\hat{U}=\frac{4\pi\hbar^2 a}{m}\delta_3(\vec{r})\frac{\partial}{\partial r}r, \tag{1}$$

where $\delta_3(\vec{r})=-(1/4\pi)\nabla^2(1/r)$ is the Dirac δ function in 3D space. This pseudopotential operator is the key to study the interaction effects on BEC, therefore, we think it deserves further investigations. In this paper, expression (1) is extended from 3D space to any-dimensional space.

In considering the case of d-dimensional space, we may use the traditional method of coordinate transformation to transform the two-body interacting problem into a single-body problem with an interacting potential. The actual two-body Hamiltonian is given by

$$\hat{H}(\vec{r}_1,\vec{r}_2)=-\frac{\hbar^2}{2m}(\nabla_1^2+\nabla_2^2)+u(\vec{r}_1-\vec{r}_2), \tag{2}$$

where

$$u(\vec{r}_1-\vec{r}_2)=\begin{cases}+\infty & \text{for} \quad |\vec{r}_1-\vec{r}_2|\leqslant a,\\ 0 & \text{for} \quad |\vec{r}_1-\vec{r}_2|>a.\end{cases} \tag{3}$$

In terms of the center-of-mass coordinates $\vec{R}=(\vec{r}_1+\vec{r}_2)/2$ and the relative coordinates $\vec{r}=\vec{r}_2-\vec{r}_1$, we have

$$\frac{\partial^2}{\partial r_{1,i}^2}=\frac{1}{4}\frac{\partial^2}{\partial R_i^2}-\frac{\partial^2}{\partial R_i\partial r_i}+\frac{\partial^2}{\partial r_i^2} \tag{4}$$

and

$$\frac{\partial^2}{\partial r_{2,i}^2}=\frac{1}{4}\frac{\partial^2}{\partial R_i^2}+\frac{\partial^2}{\partial R_i\partial r_i}+\frac{\partial^2}{\partial r_i^2}, \tag{5}$$

where $r_{1,i}$ and $r_{2,i}$ are the ith rectangular components of $\vec{r}_1$ and $\vec{r}_2$, respectively. Expressions (4) and (5) give $\nabla_1^2+\nabla_2^2=(1/2)\nabla_R^2+2\nabla_r^2$, thus the two-body wave function may be written as $\Psi(\vec{R},\vec{r})=\psi(\vec{r})\exp[i(\vec{P}\cdot\vec{R})/\hbar]$, and the eigenvalue equation for the relative motion being

$$\left\{-\frac{\hbar^2}{m}\nabla_r^2+u(\vec{r})\right\}\psi(\vec{r})=\varepsilon\psi(\vec{r}). \tag{6}$$

Noticing the hard-sphere interaction described in Eq. (3), and writing $\varepsilon=\hbar^2k^2/m$, Eq. (6) turns out to be

$$(\nabla_r^2+k^2)\psi(\vec{r})=0 \quad \text{for} \quad |\vec{r}|>a, \tag{7}$$

$$\psi(\vec{r})=0 \quad \text{for} \quad |\vec{r}|\leqslant a. \tag{8}$$

Thus the hard-sphere interaction in d-dimensional space is expressed as a boundary condition for the relative-motion wave function just as what was done in 3D space. In spherical coordinates in d-dimensional space, a vector is denoted by $\vec{r}=(r,\theta_1,\theta_2,\ldots,\theta_{d-1})\equiv(q_1,q_2,q_3,\ldots,q_d)$. The coordinate transformation gives

$$\nabla^2=\frac{1}{\prod_{i=1}^{d}M_i}\sum_{j=1}^{d}\left[\frac{\partial}{\partial q_j}\left(\frac{\prod_{i=1}^{d}M_i}{M_j^2}\frac{\partial}{\partial q_j}\right)\right], \tag{9}$$

where

$$M_i=\left[\sum_{j=1}^{d}\left(\frac{\partial x_j}{\partial q_i}\right)^2\right]^{1/2} \tag{10}$$

are the Lame coefficients. The properties of spherical coordinates result in

$$M_1=1, \tag{11}$$

$$\frac{1}{\prod_{i=1}^{d}M_i}\frac{\partial}{\partial r}\left(\frac{\prod_{i=1}^{d}M_i}{M_1^2}\frac{\partial}{\partial r}\right)=\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial}{\partial r}\right) \tag{12}$$

and

$$\frac{1}{\prod_{i=1}^{d}M_i}\frac{\partial}{\partial q_j}\left(\frac{\prod_{i=1}^{d}M_i}{M_j^2}\frac{\partial}{\partial q_j}\right)=\frac{1}{r}f_j(\theta_1,\theta_2,\cdots,\theta_{d-1})$$

$$\text{for all}\quad j\neq 1. \tag{13}$$

Consequently, expression (9) takes the form

$$\nabla^2=\frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(r^{d-1}\frac{\partial}{\partial r}\right)+\frac{1}{r}F(\theta_1,\theta_2,\ldots,\theta_{d-1}). \tag{14}$$

The actual expressions of $f_j(\theta_1,\theta_2,\ldots,\theta_{d-1})$ and $F(\theta_1,\theta_2,\ldots,\theta_{d-1})$ in Eqs. (13) and (14) are not used when deriving a spherically symmetric low-energy solution of the relative-motion wave function. Equations (7) and (8) that describe the relative-motion wave function have a spherically symmetric low-energy solution

$$\psi(\vec{r})=Y(r)=\text{const}\times\left(1-\frac{a^{d-2}}{r^{d-2}}\right). \tag{15}$$

When being applied to d-dimensional space, the Gaussian theorem gives a corresponding Dirac δ function

$$\delta_d(\vec{r})=-\frac{\Gamma(d/2+1)}{d(d-2)\pi^{d/2}}\nabla^2\frac{1}{r^{d-2}}, \tag{16}$$

where $\Gamma(x)$ is the gamma function. Expressions (14)-(16) result in

$$\nabla^2 Y=\frac{d\pi^{d/2}}{\Gamma(d/2+1)}\frac{a^{d-2}}{r^{d-3}}\delta_d(\vec{r})\frac{\partial}{\partial r}(r^{d-2}Y). \tag{17}$$

Therefore, the pseudopotential operator is formulated as

$$\hat{U}=\frac{\hbar^2}{m}\frac{d\pi^{d/2}}{\Gamma(d/2+1)}\frac{a^{d-2}}{r^{d-3}}\delta_d(\vec{r})\frac{\partial}{\partial r}r^{d-2}. \tag{18}$$

Expression (18) is a unified pseudopotential operator for the hard-sphere interaction in any-dimensional space, and may readily be reduced to Eq. (1) in 3D space as long as one takes $d=3$.

In 2D space, the pseudopotential operator reads

$$\hat{U}=\frac{2\pi\hbar^2}{m}r\,\delta_2(\vec{r})\frac{\partial}{\partial r}, \tag{19}$$

where the corresponding Dirac δ function takes the form $\delta_2(\vec{r})=(1/2\pi)\nabla^2\ln r$. If Eq. (18) is simplified for $d=2$, it comes out to be exactly Eq. (19). Thus the pseudopotential operator (18) may also be used to describe the hard-sphere interaction in 2D space. The factor $\partial/\partial r$ is nought when it acts on an unperturbed wave function, so in the low temperature and density conditions and accurate to the order a, the pseudopotential in 2D space is zero. This is in accordance with Refs. [18,19] in that the pseudopotential vanishes in 2D space, whereas Refs. [18,19] further show that the pseudopotential has a small factor $-(\ln na^2)^{-1}$ and diminishes in the limit of small na^2.

In 1D space, the pseudopotential operator (18) reduces to

$$\hat{U}=-\frac{2\hbar^2}{ma}\delta_1(\vec{r}) \tag{20}$$

and coincides with the result in literature (see, for example, Ref. [20]). Thus the pseudopotential operator (18) is also valid in the case of 1D space. In reducing Eq. (18) to Eq. (20), one should take $d=1$, and notice the symmetry of the low-energy relative-motion wave function. It is interesting that in 1D space, the pseudopotential is proportional to $-1/a$, in contrast with $\hat{U}\propto a$ in 3D space. This again is a characteristic of the 1D space.

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